

Description of Additional Supplementary Files

File Name: Supplementary Data 1

Description: Ce (cerium) – Atomic coordinates for the optimized structures of the pristine Ce–N–C single-atom catalyst and the adsorption configurations with *I, *I₂, and *I₃ species.

File Name: Supplementary Data 2

Description: Co (cobalt) – Atomic coordinates for the optimized structures of the pristine Co–N–C single-atom catalyst and the adsorption configurations with *I, *I₂, and *I₃ species.

File Name: Supplementary Data 3

Description: Cu (copper) – Atomic coordinates for the optimized structures of the pristine Cu–N–C single-atom catalyst and the adsorption configurations with *I, *I₂, and *I₃ species.

File Name: Supplementary Data 4

Description: Fe (iron) – Atomic coordinates for the optimized structures of the pristine Fe–N–C single-atom catalyst and the adsorption configurations with *I, *I₂, and *I₃ species.

File Name: Supplementary Data 5

Description: La (lanthanum) – Atomic coordinates for the optimized structures of the pristine La–N–C single-atom catalyst and the adsorption configurations with *I, *I₂, and *I₃ species.

File Name: Supplementary Data 6

Description: Mo (molybdenum) – Atomic coordinates for the optimized structures of the pristine Mo–N–C single-atom catalyst and the adsorption configurations with *I, *I₂, and *I₃ species.

File Name: Supplementary Data 7

Description: Nb (niobium) – Atomic coordinates for the optimized structures of the pristine Nb–N–C single-atom catalyst and the adsorption configurations with *I, *I₂, and *I₃ species.

File Name: Supplementary Data 8

Description: Sm (samarium) – Atomic coordinates for the optimized structures of the pristine Sm–N–C single-atom catalyst and the adsorption configurations with *I, *I₂, and *I₃ species.

File Name: Supplementary Data 9

Description: V (vanadium) – Atomic coordinates for the optimized structures of the pristine V–N–C single-atom catalyst and the adsorption configurations with *I, *I₂, and

*I₃ species.

File Name: Supplementary Data 10

Description: W (tungsten) – Atomic coordinates for the optimized structures of the pristine W–N–C single-atom catalyst and the adsorption configurations with *I, *I₂, and *I₃ species.

File Name: Supplementary Data 11

Description: Zr (zirconium) – Atomic coordinates for the optimized structures of the pristine Zr–N–C single-atom catalyst and the adsorption configurations with *I, *I₂, and *I₃ species.